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HOT PLASMAS

D. B. Boercker, K. Warren
and
G. Haggin

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ION DIFFUSION AT INTERFACES IN HOT PLASMAS*

D. B. Boercker, K. Warren and G. Haggin

University of California, Lawrence Livermore National Laboratory
Livermore, California 94550

Abstract

There are many laboratory applications in which it is important to know how fast two hot, ionized materials mix across an initially sharp interface. The speed of this process is regulated by the interdiffusion coefficient for the species involved. In a previous work, a theoretical method for calculating the interdiffusion coefficient in a Binary Ionic Mixture (classical ions in a uniform, neutralizing background) was described and found to give excellent agreement with Molecular Dynamics estimates. The purpose of this report is to show how these results may be applied to a model of the plasma interface, including electric field effects, to give a good description of the mixing across it.

Introduction

In Ref. 1, the ions in a binary plasma mixture were modeled as an effective two-component system of classical ions moving in a uniform, neutralizing background of electrons. This model is referred to as the Binary Ionic Mixture. In a very similar model, the electrons are allowed to respond to the ions so that the effective ion-ion interaction is a Coulomb potential screened by the electron Debye length $\lambda_e = (k_B T / 4 e^2 n_e)^{1/2}$.

A possible difficulty with both models is that they do not explicitly account for the electric field effects due to the presence of the electrons. As is well known, from the theory of ambipolar diffusion, such fields can cause significant enhancement of ion diffusion.² It should be noted, however, that traditional ambipolar diffusion occurs in very slightly ionized plasmas in which the diffusion process is dominated by collisions with neutrals. In the plasma of interest here, there are no neutrals and the electron density is very high. As a result, the electrons may be assumed to be in (quasi) equilibrium with the relatively slowly developing ion distribution, and since $\lambda_e \sim 10$ Angstroms the plasma may be considered to be neutral over hydrodynamic scale lengths (microns). Therefore, one might expect the effects of the ambipolar field to be somewhat different in dense plasmas. We will begin our investigation of this question by reviewing the principal results of Ref. 1.

The diffusion coefficient, D , in a binary mixture linearly relates the diffusion current to the gradient of the mass concentration.

$$\vec{j}_1 \equiv m_1 n_1 (\vec{u}_1 - \vec{u}) = -\rho D \vec{\nabla} X_1 \quad (1)$$

In the above m_i is the mass of a particle of species "i", n_i is the number density of that species, \vec{u} is the mass averaged (center-of-mass) velocity field, ρ is the total mass density, and $X_i = m_i n_i / \rho$ is the mass concentration of "i". The time and position dependence of all these functions has been suppressed. It was shown in Ref. 1 that in a BIM, the diffusion coefficient may be written as

$$D = \left(\frac{c_1 c_2}{S_{cc}(k=0)} \right) \frac{3}{8} \left(\frac{2}{\pi} \right)^{1/2} \frac{(k_B T)^{5/2}}{(n_1 + n_2) \mu_{12}^{1/2} Z_1^2 Z_2^2 e^4 \Lambda} \equiv F D_0 \quad (2)$$

where $Z_1 e$ and $Z_2 e$ are the charges of the ions, the number concentration of species "i" is $c_i = n_i / (n_1 + n_2)$, μ_{12} is the reduced mass of the ions, and Λ is a generalization of the Coulomb logarithm which remains valid even in very dense plasmas.¹

The function $S_{cc}(k)$ is the concentration structure factor, defined in terms of partial structure factors by,³

$$S_{cc}(k) = c_1 c_2 (c_2 S_{11}(k) + c_1 S_{22}(k) - 2 (c_1 c_2)^{1/2} S_{12}(k)) \quad (3)$$

The factor, F , is defined by

$$F = c_1 c_2 / S_{cc}(k=0) \quad (4)$$

When either concentration vanishes $F=1$, and for all intermediate concentrations $F>1$, so it represents an enhancement of the diffusion predicted by D_0 , alone. For future reference, we note that in a screened BIM, the Debye-Hückel limit of F is

$$F \rightarrow \frac{\langle Z^2 \rangle + \langle Z \rangle}{\langle Z \rangle^2 + \langle Z \rangle} \quad (5)$$

where $\langle A \rangle = c_1 A_1 + c_2 A_2$. Usually, this factor is not large, but it can be quite significant if one charge is much greater than the other.

In the next section, we will demonstrate the connection between the factor, F , and the ambipolar field by starting with the usual Boltzmann theory of diffusion in a three-component system (two ion species plus electrons). The result will be to show that under the conditions of local neutrality and equilibrium for the electrons, the ambipolar fields enhance the ion diffusion by precisely the factor in Eq. (5). While strictly valid only in the low

density limit, this argument indicates that it is reasonable to model the ions as an effective two-component system with the ambipolar effects implicitly contained in the enhancement factor.

Diffusion in Multicomponent Systems and the Ambipolar Field

The generalization of Eq. (1) to a three-component system in which there are no temperature gradients is,⁴

$$\vec{j}_i = \sum_{j=1}^3 \frac{m_i m_j n}{\rho} D_{ij} \vec{d}_j \quad (6)$$

where the D_{ij} 's are the multicomponent diffusion constants, ($D_{ii} = 0$), $n = n_1 + n_2 + n_3$, and

$$\vec{d}_j = \frac{1}{n} (\vec{V} n_j - \frac{n_j}{k_B T} \vec{F}_j) + \frac{m_i n_i}{\rho n k_B T} \left(\sum_{j=1}^3 n_j \vec{F}_j - \nabla p \right) \quad (7)$$

The forces in Eq. (7) are due to the ambipolar field, and the pressure, p , has been assumed to be given by the ideal gas law. If one assumes mechanical stability for the system, then

$$\sum_{j=1}^3 n_j \vec{F}_j = \vec{V} p \quad (8)$$

and Eq. (5) reduces to,

$$\vec{d}_j = \frac{1}{n} \left(\vec{V} n_j - \frac{z_j n_j e}{k_B T} \vec{E} \right) \quad (9)$$

where \vec{E} is the electric field.

If we choose the label "3" to represent the electrons and assume them to be in local equilibrium, then

$$\vec{v}_{n_3} = \frac{-en_3}{k_B T} \vec{E} = \frac{Z_3 n_3}{k_B T} \vec{E} \quad (10)$$

and d_3 vanishes. As a result the diffusion current for ion species "1" is given by only the single term,

$$\vec{j}_1 = \frac{m_1 m_2 n^2}{\rho} D_{12} \vec{d}_2 = \frac{m_1 m_2 n}{\rho} D_{12} \left(\vec{v}_{n_2} + \frac{Z_2 n_2}{n_3} \vec{v}_{n_3} \right) \quad (11)$$

From local neutrality, and Eq. (8), it follows that,

$$\vec{v}_{n_3} = \frac{(Z_1 - Z_2)}{Z_2 + 1} \vec{v}_{n_1} \quad (12)$$

and

$$\vec{v}_{n_2} = \frac{-(Z_1 + 1)}{(Z_2 + 1)} \vec{v}_{n_1} \quad (13)$$

Hence, we obtain,

$$\vec{j}_1 = - \frac{m_1 m_2 n}{\rho (Z_2 + 1)} D_{12} \frac{\langle Z^2 \rangle + \langle Z \rangle}{\langle Z \rangle} \vec{v}_{n_1} \quad (14)$$

Since the electron contribution to the mass density is negligible, we relate the gradient of n_1 to that of x_1 through

$$\vec{v}_{n_1} = \frac{\rho^2}{m_1 m_2} \frac{1}{n_1 + n_2} \frac{(Z_2 + 1)}{\langle Z \rangle + 1} \vec{v}_{x_1} \quad (15)$$

and we obtain

$$\vec{j}_1 = - \rho \left(\frac{n}{n_1 + n_2} D_{12} \right) \frac{\langle Z^2 \rangle + \langle Z \rangle}{\langle Z \rangle^2 + \langle Z \rangle} \vec{v}_{x_1} \quad (16)$$

It remains only to connect the multicomponent diffusion constant, D_{12} to the binary diffusion constant in Eq. (2). Once again exploiting the smallness of the electron mass we obtain,⁴

$$D_{12} = \frac{3}{8} \left(\frac{2}{\pi}\right)^{1/2} \frac{(k_B T)^{5/2}}{n \mu_{12}^{1/2} Z_1^2 Z_2^2 e^4 \Lambda_c} \quad (17)$$

where Λ_c is the Coulomb logarithm. Comparing with Eq. (2) we see that,

$$D_{12} \approx \frac{n_1 + n_2}{n} D_0 \quad (18)$$

So, we obtain

$$\vec{j}_1 = - \rho \left(D_0 \frac{\langle Z^2 \rangle + \langle Z \rangle}{\langle Z \rangle^2 + \langle Z \rangle} \right) \vec{\nabla} \cdot \vec{x}_1 \quad (19)$$

The important point to make here is that the enhancement factor appearing in Eq. (19) is identical to that in Eq. (5). Thus modeling the true three-component system of electrons and ions as an effective two-component system of screened ions is legitimate provided the enhancement factor is included.

Numerical Results

The general problem of diffusion is greatly simplified under conditions, such as those considered here, in which the total number density is a constant.⁴ In this case the number averaged velocity, \vec{w} , can be shown to have no divergence. By adding the continuity equations for each species, we obtain,

$$\frac{\partial n}{\partial t} = - \vec{\nabla} \cdot (n \vec{w}) = - n (\vec{\nabla} \cdot \vec{w}) = 0 \quad (20)$$

If one assumes that \vec{w} is also irrotational, then \vec{w} must be independent of the spatial coordinates. To make use of this fact we write the continuity equation for ion species "1" as,

$$\frac{\partial n_1}{\partial t} = -\nabla \cdot n_1 (\vec{u}_1 - \vec{w}) - \vec{w} \cdot \vec{\nabla} n_1 \quad (21)$$

Since charge neutrality requires that the electron velocity be given by,

$$n_3 \vec{u}_3 = z_1 n_1 \vec{u}_1 + z_2 n_2 \vec{u}_2 \quad (22)$$

we obtain

$$\begin{aligned} n_1 (\vec{u}_1 - \vec{w}) &= n_1 \left(\vec{u}_1 - \frac{n_1 \vec{u}_1 + n_2 \vec{u}_2 + n_3 \vec{u}_3}{n} \right) \\ &= \frac{n_1 n_2}{n} (z_2 + 1) (\vec{u}_1 - \vec{u}_2) \end{aligned} \quad (23)$$

Once again neglecting electron mass effects, we can write Eq. (14) in the form

$$\vec{u}_1 - \vec{u}_2 = -D \frac{n}{(z_2 + 1) n_1 n_2} \vec{\nabla} n_1 \quad (24)$$

where the enhancement factor is included in D. Substituting Eqs. (20,21) into Eq. (18) leads to,

$$\frac{\partial n_1}{\partial t} = \nabla \cdot D \vec{\nabla} n_1 - \vec{w} \cdot \vec{\nabla} n_1 \quad (25)$$

which for $\vec{w} = 0$ is just Fick's law.⁴

We have written a code that solves Eq. (25), with $\vec{w} = 0$, using the implicit differencing scheme described in Ref. 5. The diffusion coefficient is calculated from Eq. (2) with Λ evaluated from the theory in Ref. 1, and read into the code in tabular form. The enhancement factor is estimated at each point from Eq. (5).

Figure 1 shows results for silicon and strontium at 1 keV in planar geometry. The interface was initially sharp at $x = 0$, and after 5 ns, it

appears to be about 2 microns thick. The thinner lines indicate the diffusion predicted with Λ replaced by the estimate $\Lambda \rightarrow \Lambda_g \equiv \text{Max} [1., \Lambda_c]$.

The spreading of the interface in this case is much less, because the value of Λ calculated from Ref. 1 is typically about 0.2.

In Fig. 2, we solve Eq. (25) in spherical geometry. The initial conditions are designed to simulate a micron diameter bubble of Sr in a Si background. We see that after about 5 ns, the bubble has significantly evaporated.

Summary

We have demonstrated that if the ions in a dense plasma are modelled as an effective binary mixture, the effects of the ambipolar field are implicitly contained in the enhancement factor,

$$F = \frac{c_1 c_2}{S_{cc}(k=0)} \approx \frac{\langle Z^2 \rangle + \langle Z \rangle}{\langle Z \rangle^2 + \langle Z \rangle} \quad (25)$$

where S_{cc} is the concentration correlation function. A small computer code has been written that solves the diffusion equation using estimates of the effective Coulomb logarithm from the theory described in Ref. 1. Typical results from that code in both planar and spherical geometry have been presented for mixtures of Si and Sr.

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FIGURE CAPTIONS

- FIG. 1** Planar Si-Sr interface shown at a) $t = 0$ and b) $t = 5$ nsecs. The thinner lines in b) represent diffusion calculated with a Spitzer-like theory.
- FIG. 2** Spherical Si-Sr interface shown at a) $t = 0$, b) $t = 2$ nsecs. and c) $t = 5$ nsecs.

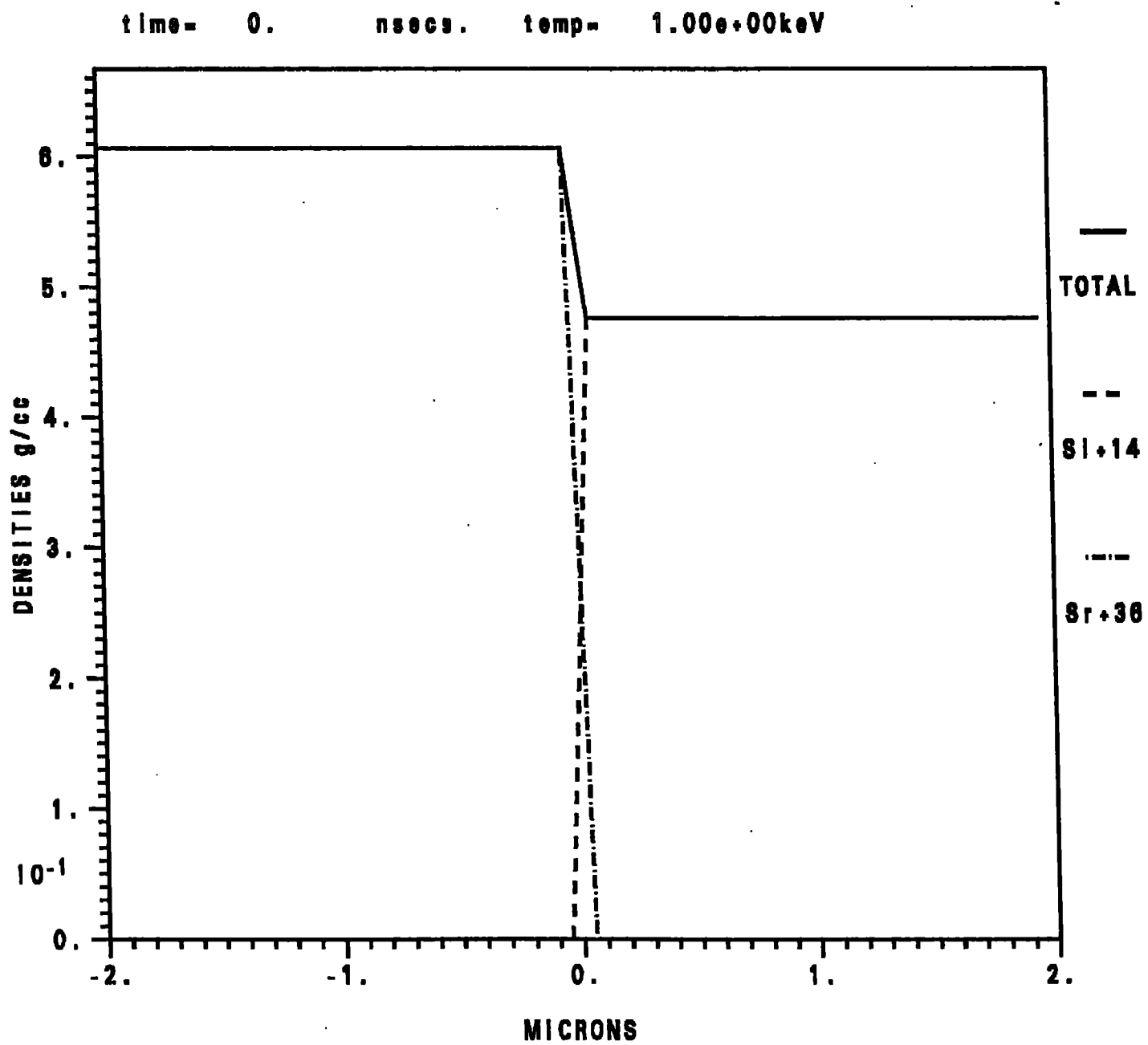


Fig. 1a

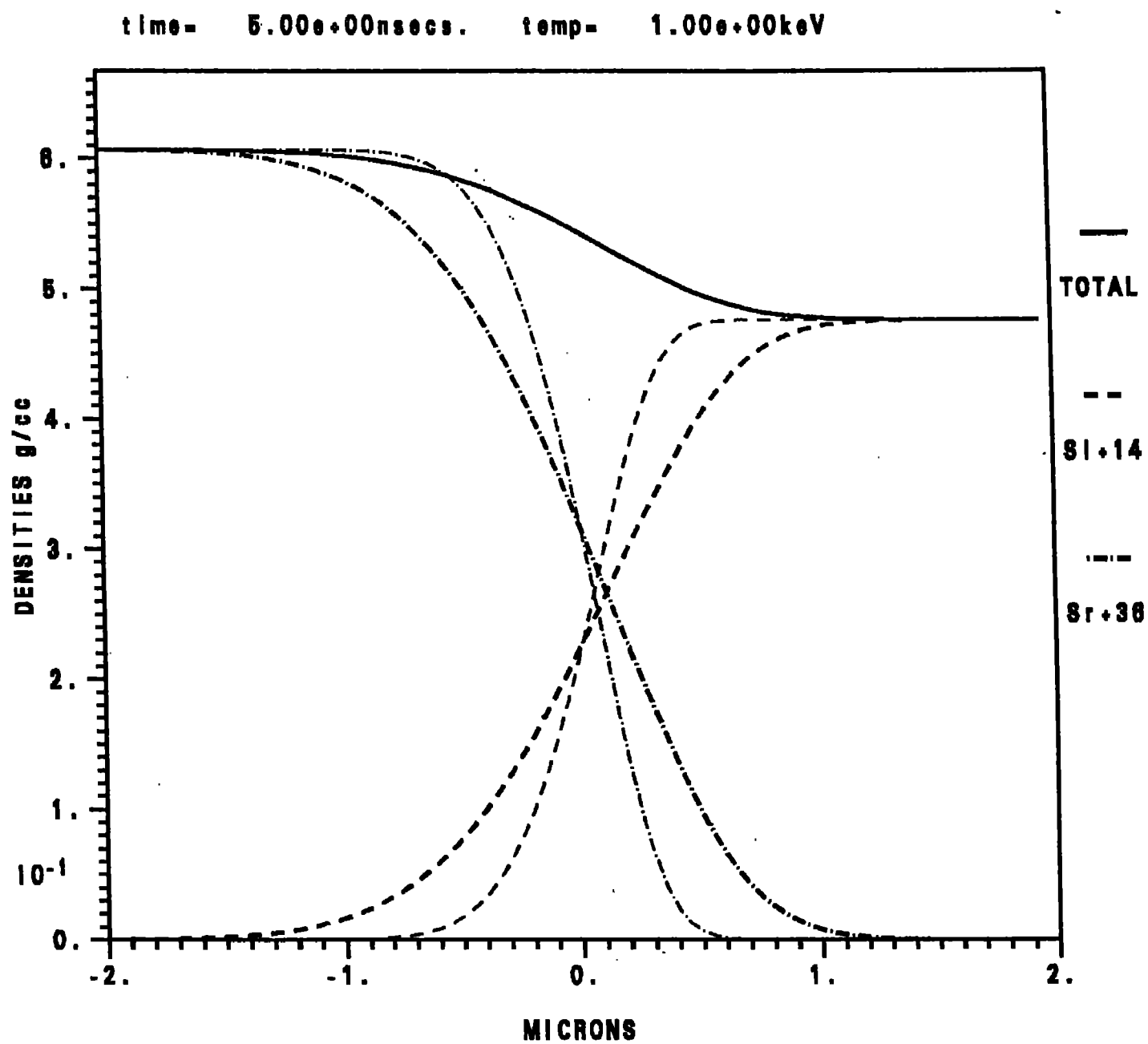


Fig. 1b

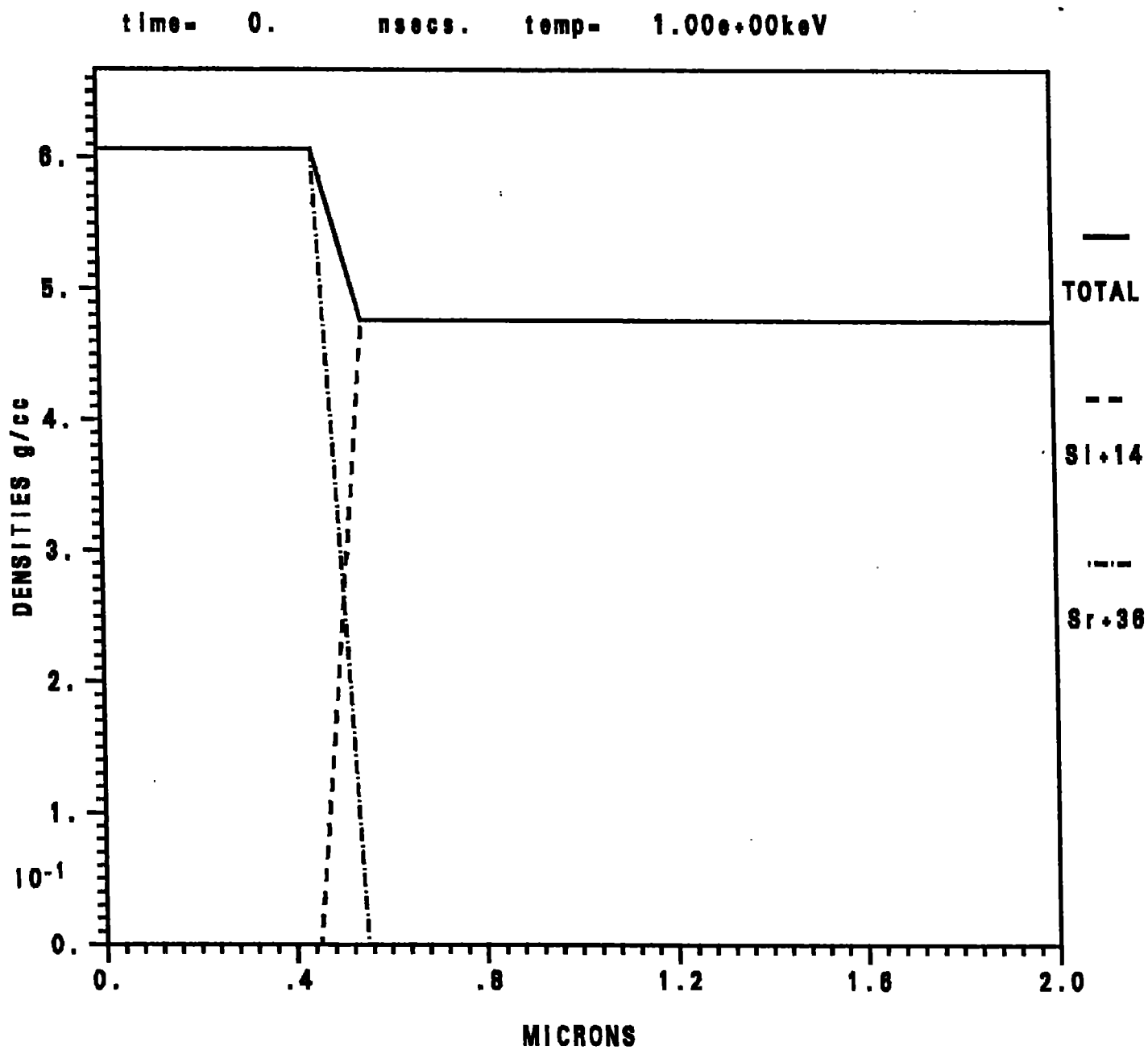


Fig. 2a

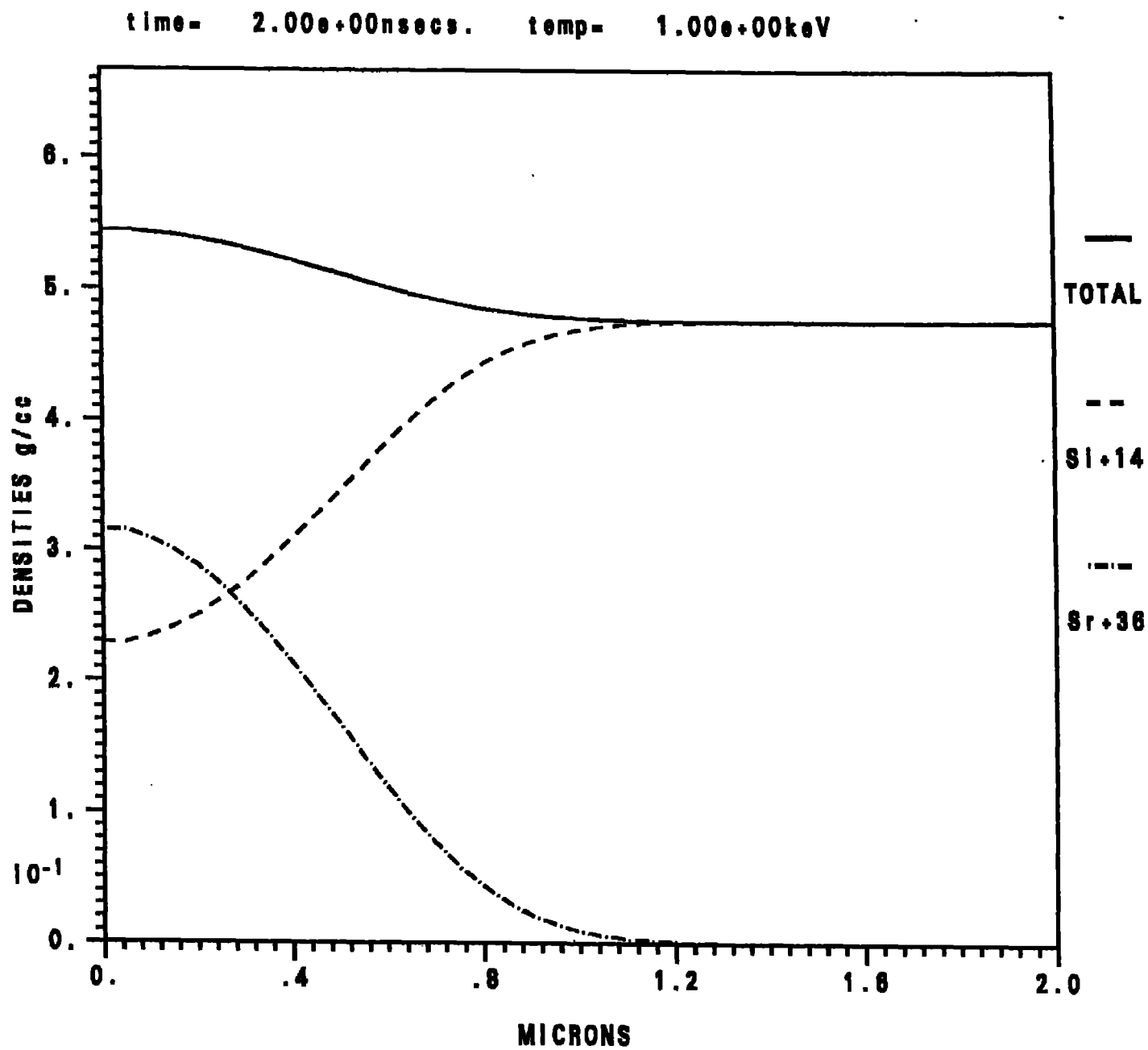


Fig. 2b

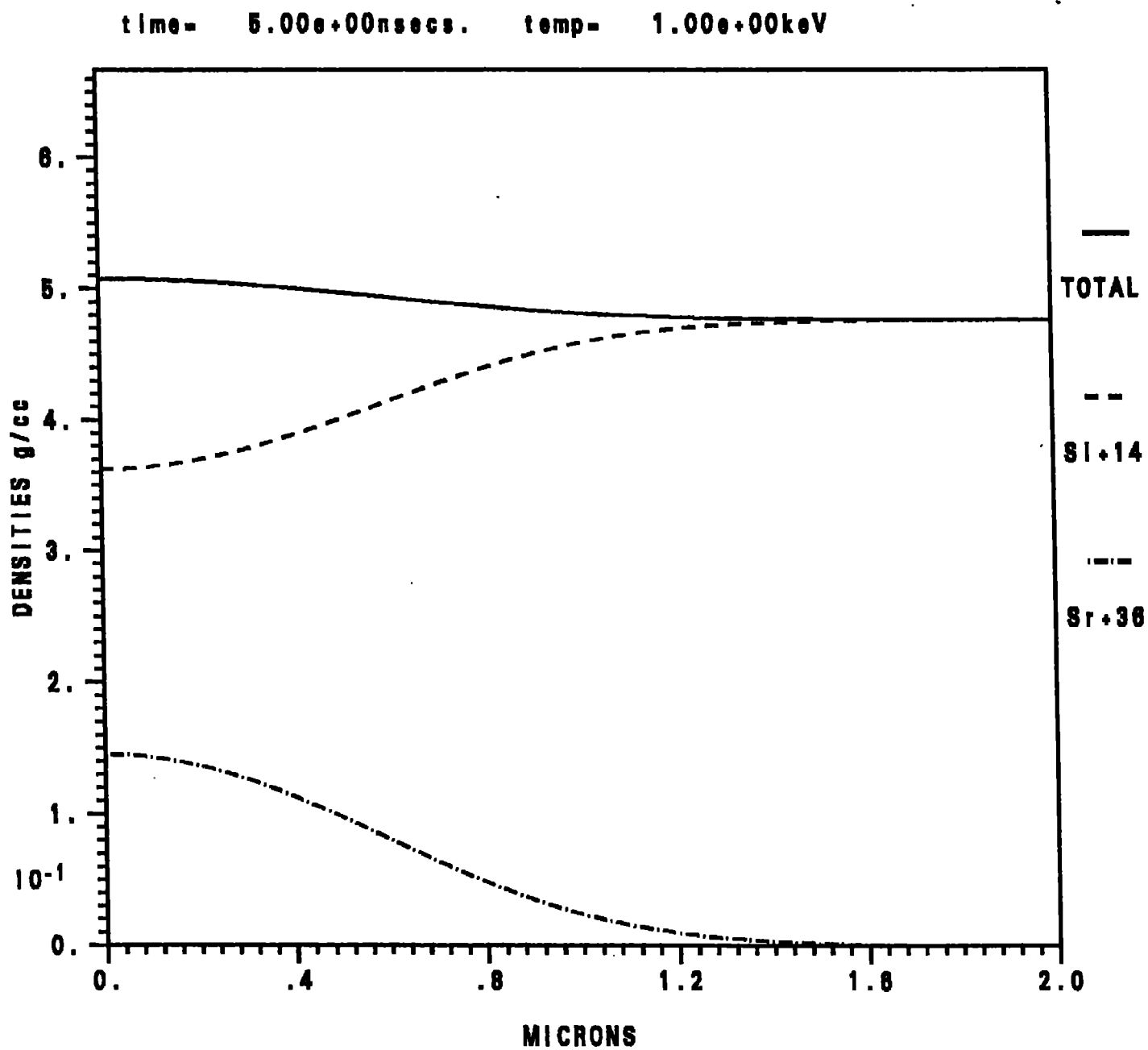


Fig. 2c